Analysis of the thermomechanical inconsistency of some extended hydrodynamic models at high Knudsen number

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There are some hydrodynamic equations that, while their parent kinetic equation satisfies fundamental mechanical properties, appear themselves to violate mechanical or thermodynamic properties. This paper aims to shed some light on the source of this problem. Starting with diffusive volume hydrodynamic models, the microscopic temporal and spatial scales are first separated at the kinetic level from the macroscopic scales at the hydrodynamic level. Then, we consider Klimontovich's spatial stochastic version of the Boltzmann kinetic equation and show that, for small local Knudsen numbers, the stochastic term vanishes and the kinetic equation becomes the Boltzmann equation. The collision integral dominates in the small local Knudsen number regime, which is associated with the exact traditional continuum limit. We find a subdomain of the continuum range, which the conventional Knudsen number classification does not account for appropriately. In this subdomain, it is possible to obtain a fully mechanically consistent volume (or mass) diffusion model that satisfies the second law of thermodynamics on the grounds of extended non-local-equilibrium thermodynamics.

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I. INTRODUCTION

The Boltzmann kinetic equation is the standard model for dilute gas flows [1]. In its kinetic structure, a molecular spatial displacement is presented as a deterministic drift motion. Approximate solutions to the Boltzmann equation are known to recover the Navier-Stokes-Fourier model for continuum fluid mechanics. However, "in a gas in which finite departures from equilibrium are imposed by forces too strong or too rapid to be overcome by collisions, a satisfactory comparison between kinetic theory and experiments is much harder to achieve" [2].

Some criticisms of the original Boltzmann model have led to various proposals for modifications, for example, incorporating a spatial stochastic term [3–5]. In the subsequent continuum-fluid set of partial differential equations, a spatial stochastic term in the kinetic model results in an additional mass or volume diffusive term. This term has always been a source of controversy (see, for example, a review in Ref. [3]). Paradoxically, however, when applied to some noncontinuum flows, it appears that a diffusive volume-mass model can capture some noncontinuum flow behavior and can resolve some observed paradoxes [3,6–10]. Considering the derivation of dissipative volume-mass models in the General Equation for the NonEquilibrium Reversible-Irreversible Coupling formalism [11], Öttinger *et al*. found there to be incompatibilities however with some fundamental mechanical principles—the most important being local angular momentum conservation [12]. The family of dissipative volume-mass models investigated in that case was founded on the assumption of local equilibrium [13].

In fact, there is an entire class of hydrodynamic models where, even though the parent kinetic equation appears not to have any mechanical inconsistency, the associated macroscopic sets of equations do appear mechanically inconsistent. Typical examples include the class of high order hydrodynamics models obtained as terms beyond Navier-Stokes-Fourier order when approximating the original Boltzmann kinetic equation [14–17].

The purpose of the present paper is to show that there exists a subcontinuum fluid domain that is not properly accounted for by the traditional Knudsen number classification. This subcontinuum domain seems to coincide with the traditional slip and transition regimes in which matches between experiments and theory have always been difficult to achieve. A volume-mass diffusion appears to lie within that domain of non-local-equilibrium flows.

II. AN EXAMPLE OF A DISSIPATIVE VOLUME-MASS MODEL AND ITS INCONSISTENCIES

We consider the following spatial stochastic kinetic model, which can be derived in different ways [4,18]:

$$\frac{\partial f}{\partial t} + \xi \cdot \nabla f - \nabla \cdot \kappa \nabla f + F_{\text{ext}} \cdot \nabla_\xi f - I_\xi(f,f) = 0, \qquad (1)$$

where $f \equiv f(t,X,\xi)$ is the molecular distribution function that depends on time t, molecular velocity ξ, and position X. The term denoted $I_\xi(f,f)$ is the Boltzmann collision integral. Compared with the Boltzmann kinetic model of a dilute gas, the difference is the third term on the left-hand side. This is a molecular spatial diffusion term that arises when accounting for spatial stochasticity in the kinetic description [4]. The coefficient κ is then a spatial diffusion coefficient. In our notation in this section, ∇ denotes the spatial gradient operator and ∇_ξ denotes the gradient operator in velocity space; F_{ext} represents external forces, such as gravity, but these will be neglected in this paper.

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A. Macroscopic flow properties

Macroscopic mass density $\rho(t,X)$ and macroscopic flow velocity $U(t,X)$ may be defined through,

$$\rho = \int M f(t,X,\xi) d_\xi, \tag{2}$$

and

$$\rho U = \int M \xi f(t,X,\xi) d_\xi. \tag{3}$$

Then, the peculiar velocity corresponds to

$$C = \xi - U, \tag{4}$$

so that the internal energy $e_{in}(t,X)$ and the macroscopic momentum and energy diffusion flux tensor and vectors $\mathbf{P}_{ij}(t,X)$ and $\mathbf{q}(t,X)$, respectively, can be associated via

$$\begin{aligned} \rho e_{in} &= \int \frac{1}{2} C^2 f d_\xi, \quad \mathbf{P}_{ij} = \int\int C_i C_j f d_\xi, \\ \mathbf{q} &= \int \frac{1}{2} C^2 C f d_\xi. \end{aligned} \tag{5}$$

B. A macroscopic continuum set of equations

Multiplying the stochastic kinetic equation (1) by $M, M\xi, M\xi^2/2$, and integrating over velocity space gives, respectively,

(1) Mass density,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho U \underline{- \kappa \nabla \rho}] = 0, \tag{6}$$

(2) Momentum,

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot [\rho U U] + \nabla \cdot [p\mathbf{I} + \Pi] \underline{- \nabla \cdot [\kappa \nabla (\rho U)]} = 0, \tag{7}$$

(3) Energy,

$$\begin{aligned} &\frac{\partial}{\partial t}\left[\frac{1}{2}\rho U^2 + \rho e_{in}\right] + \nabla \cdot \left[\frac{1}{2}\rho U^2 U + \rho e_{in} U\right] \\ &+ \nabla \cdot [(p\mathbf{I} + \Pi) \cdot U] + \nabla \cdot [\mathbf{q}] \\ &\underline{- \nabla \cdot \left[\kappa \nabla \left(\frac{1}{2}\rho U^2 + \rho e_{in}\right)\right]} = 0, \end{aligned} \tag{8}$$

where $\mathbf{I}$ is the identity matrix and $\Pi = \mathbf{P} - p\mathbf{I}$ with p is the kinetic pressure related to the internal energy by $3p = 2\rho e_{in}$. Compared with the conventional fluid dynamic set of conservation equations, new terms in the above set are underlined (and this formatting will be continued below). These new terms all have clear meaning from the derivation: the underlined term in the mass-density equation is a mass or volume diffusion component resulting from the random spatial distribution of molecules. The underlined terms in the momentum and energy equations are, respectively, momentum and energy diffusion resulting from the same random changes in positions at the microscopic level (not the random exchange of momentum).

The shear stress and heat flux that result from molecular-level random exchange of momentum and energy can be given their Navier-Stokes and Fourier law expressions,

$$\Pi = -\mu[\nabla U + (\nabla U)^{tr}] + \eta \nabla \cdot U \mathbf{I} \quad \text{and} \quad \mathbf{q} = -\kappa_h \nabla T, \tag{9}$$

with μ, η, and κ_h being, respectively, the dynamic and volume viscosities and the heat conductivity. Temperature T is associated, according to the kinetic theory definition, with $e_{in} = (3/2)RT$, with R being the specific gas constant.

C. The thermodynamic and mechanical inconsistencies

Assuming a material derivative denoted by $D/Dt = \partial/\partial t + U \cdot \nabla$, Eq. (7) can be rewritten

$$\begin{aligned} &\rho \frac{DU}{Dt} + \left(\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho U]\right) U \\ &+ \nabla \cdot [p\mathbf{I} + \Pi] \underline{- \nabla \cdot [\kappa \nabla (\rho U)]} = 0, \end{aligned} \tag{10}$$

which becomes, after introducing the mass-density equation (6),

$$\rho \frac{DU}{Dt} + \nabla \cdot [p\mathbf{I} + \Pi] + \underline{(\nabla \cdot [\kappa \nabla \rho]) U - \nabla \cdot [\kappa \nabla (\rho U)]} = 0. \tag{11}$$

Taking the cross product of Eq. (11) with a hydrodynamic position vector X, we notice that the underlined terms generate

$$X \wedge \{(\nabla \cdot [\kappa \nabla \rho]) U - \nabla \cdot [\kappa \nabla (\rho U)]\}, \tag{12}$$

which we cannot write in local conservative form, i.e., as $\nabla \cdot [\cdots]$. So, these terms appear as local angular momentum production terms. Equation (11) is, therefore, said to violate local angular momentum conservation [11].

To analyze the second law of thermodynamics, energy equation (8) is first re-written

$$\rho \frac{D}{Dt}\left[\frac{1}{2}U^2 + e_{in}\right] + \left(\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho U]\right)\left(\frac{1}{2}U^2 + e_{in}\right) + \nabla \cdot [(p\mathbf{I} + \Pi) \cdot U] + \nabla \cdot [\mathbf{q}] \underline{- \nabla \cdot \left[\kappa \nabla \left(\frac{1}{2}\rho U^2 + \rho e_{in}\right)\right]} = 0, \tag{13}$$

which becomes, after introducing the mass conservation equation (6),

$$\rho \frac{D}{Dt}\left[\frac{1}{2}U^2 + e_{in}\right] + \nabla \cdot [\kappa \nabla \rho]\left(\frac{1}{2}U^2 + e_{in}\right) + \nabla \cdot [(p\mathbf{I} + \Pi) \cdot U] + \nabla \cdot [\mathbf{q}] \underline{- \nabla \cdot \left[\kappa \nabla \left(\frac{1}{2}\rho U^2 + \rho e_{in}\right)\right]} = 0. \tag{14}$$

Momentum equation (11) can be used to eliminate the macroscopic kinetic energy terms; introducing the density equation (6), the energy equation is finally,

$$\rho\frac{De_{in}}{Dt}+p\rho\frac{D\rho^{-1}}{Dt}\underline{-2\kappa\nabla\rho\cdot\nabla e_{in}-\kappa\rho\nabla\cdot\nabla e_{in}+\frac{p}{\rho}\nabla\cdot[\kappa\nabla\rho]-\kappa\rho\nabla U{:}\nabla U}+\Pi{:}\nabla U+\nabla\cdot[\mathbf{q}]=0, \tag{15}$$

in which ":" denotes the Frobenius inner product. In classical fluid dynamics, the specific entropy s is defined by adopting the Gibbs (local equilibrium) equation,

$$\rho T\frac{Ds}{Dt}=\rho\frac{De_{in}}{Dt}+p\rho\frac{D\rho^{-1}}{Dt}. \tag{16}$$

Using Eq. (16), energy equation (15) becomes an equation for the entropy,

$$\rho\frac{Ds}{Dt}\underline{-\frac{\kappa c_v}{T}\nabla\cdot\nabla(\rho T)+\kappa(R+c_v)\nabla\cdot\nabla\rho-\kappa\rho\frac{1}{T}\nabla U{:}\nabla U}+\frac{1}{T}\Pi{:}\nabla U+\frac{1}{T}\nabla\cdot[\mathbf{q}]=0, \tag{17}$$

where we have used $e_{in}=c_vT$. Finally, with the identity,

$$\frac{1}{\phi}\nabla\cdot\nabla\phi=\frac{\nabla\phi\cdot\nabla\phi}{\phi^2}+\nabla\cdot\left(\frac{\nabla\phi}{\phi}\right), \tag{18}$$

where ϕ is a scalar field, the entropy equation (17) takes the form

$$\begin{aligned}\rho\frac{Ds}{Dt}&\underline{-\rho\kappa c_v\nabla\cdot\left(\frac{\nabla(\rho T)}{\rho T}\right)+\rho\kappa(R+c_v)\nabla\cdot\left(\frac{\nabla\rho}{\rho}\right)-\kappa_h\nabla\cdot\left(\frac{\nabla T}{T}\right)}\\&=\underline{\frac{\kappa\rho}{T}\nabla U{:}\nabla U}-\frac{1}{T}\Pi:\nabla U+\frac{\kappa_h+\rho\kappa c_v}{T^2}\nabla T\cdot\nabla T+\underline{\left\{\frac{2\kappa T c_v}{T^2}\nabla\rho\cdot\nabla T-\frac{\rho\kappa R}{\rho^2}\nabla\rho\cdot\nabla\rho\right\}}.\end{aligned} \tag{19}$$

The terms in curly brackets in Eq. (19) can be either negative or positive. This suggests that a negative temperature or decreasing entropy could occur. According to classical thermodynamics with the Gibbs equation (16), these terms are, therefore, undesirable. These difficult terms in both the momentum and the entropy equations are generated by the diffusive term in the density equation (or, more precisely, the spatial diffusive term in the initial kinetic equation).

Despite the problems observed with Eqs. (12) and (19), kinetic equation (1) and others of that type do admit an H theorem [3,4]. In the following sections, we demonstrate, using a scaling analysis, that the problematic terms do not actually belong to the standard vanishing Knudsen number regime.

III. A SPATIAL AND TEMPORAL SCALING PROBLEM

A. Three scaling parameters

In continuum fluid mechanics, three different spatial scaling parameters can be identified and are represented in Fig. 1.

The three scaling parameters are [19] as follows:

(1) the molecular mean-free path λ,
(2) the length scale of the local element of fluid volume l_{loc},
(3) the macroscopic flow length scale L.

Classical continuum theory assumes the following systematic ordering:

$$\lambda\ll l_{\rm loc}\ll L. \tag{20}$$

However, in order to resolve typical non-local-equilibrium effects, for example, in rarefied gases confined in a microdevice, requires a different ordering,

$$l_{\rm loc}<\lambda\ll L, \tag{21}$$

or

$$l_{\rm loc}\ll L<\lambda. \tag{22}$$

Ordering (20) means sufficient collisions take place to assure a local thermodynamic equilibrium in the volume element $l_{\rm loc}^3$. In the order (21), molecular collisions are rare and insufficient to assure a local equilibrium. So, we may define a local Knudsen number $K_{n_{\rm loc}}$, and the conventional Knudsen number K_n, as follows:

$$K_{n_{\rm loc}}=\frac{\lambda}{l_{\rm loc}}\quad\text{and}\quad K_n=\frac{\lambda}{L}, \tag{23}$$

which characterize different types of relaxation processes: whereas K_n is used to classify the degree of nonequilibrium related to collisions, $K_{n_{\rm loc}}$ is related to relaxation processes not necessarily controlled by collisions. Order (22) can simply be

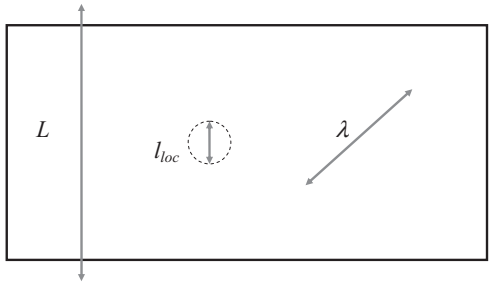

FIG. 1. Schematic of the three classical scaling parameters in gases.

viewed as the free molecular flight regime in which continuum fluid modeling becomes completely inappropriate. So taking a continuum limit, in the classical sense, as the regime where $l_{\rm loc} \ll L$, we observe that there are still two subcontinuum domains to be distinguished: $\lambda < l_{\rm loc}$ and $l_{\rm loc} < \lambda$. We contend that the controversies surrounding volume-mass diffusion, for example, arise in the latter case where there may be relaxation processes not related to intermolecular collisions.

B. Resolving the spatial and temporal scaling problems

First, we note that kinetic equation (1) is written for molecular motions and distributions. Second, it is admitted that, in writing the Boltzmann kinetic equation, the drift term $\xi \cdot \nabla f$ describes a deterministic molecular motion. From this viewpoint, the position variable involved in kinetic equations, such as Eq. (1), with its associated gradient operator ∇, refers to a molecular spatial position. However, the position variable involved in macroscopic field variables [for example, the macroscopic density $\rho(t,X)$] corresponds to a different scale.

This view of a scale difference between the molecular and the macroscopic or hydrodynamic interpretations of the position variable is shared by a number of researchers [3,11,15,20–22]. Here, we start to account for this difference by re-denoting the molecular position variable as x and the macroscopic continuum position variable as X. The associated gradient operator for the microscopic level will be denoted ∇_x, whereas ∇ will denote the gradient using the macroscopic spatial variable. Scaling molecular to macroscopic position variables requires us to recognize that the characteristic length scale associated with the molecular position variable x should be $l_{\rm loc}$ (and not L). We, therefore, set $X = \epsilon x$ with $\epsilon = K_{n_{\rm loc}}$.

The two different gradient operators follow accordingly:

$$\nabla_x = \epsilon \nabla \quad \text{and} \quad \nabla_x \cdot \nabla_x = \epsilon^2 \nabla \cdot \nabla. \tag{24}$$

Time variables and associated derivatives should also be distinguished at the different scales,

$$t = \varepsilon \tau \quad \text{and} \quad \frac{\partial}{\partial \tau} = \varepsilon \frac{\partial}{\partial t}, \tag{25}$$

with τ as the microscopic and t as the macroscopic time scales; ε may also be viewed as a Knudsen number as it is the ratio of molecular to macroscopic relaxation times. In flows with speeds typically on the same order of magnitude as the molecular speed, we can adopt $\varepsilon = \epsilon$. Sound wave propagation is such an example (and volume-mass diffusion models have been shown to give surprisingly good predictions for this [8]). More generally, Eqs. (24) and (25) can be interpreted as accounting for the observation that changes at the molecular spatial length scale do not occur at the same rate as changes at the macroscopic continuum spatial scale.

C. Re-interpretation of the dissipative volume-mass kinetic equation

Now that we are distinguishing between molecular and macroscopic time and space variables, the distribution function at the molecular level is written $f \equiv f(\tau, x, \xi)$. So, the new kinetic equation, from rewriting Eq. (1), is as follows:

$$\frac{\partial f}{\partial \tau} + \xi \cdot \nabla_x f - \nabla_x \cdot \kappa \nabla_x f - I_\xi(f,f) = 0, \tag{26}$$

from which, after substituting the changes in time and spatial variables from Eqs. (24) and (25), we obtain

$$\varepsilon \frac{\partial \bar{f}}{\partial t} + \epsilon \xi \cdot \nabla \bar{f} - \epsilon^2 \nabla \cdot \kappa \nabla \bar{f} - I_\xi(\bar{f},\bar{f}) = 0, \tag{27}$$

where $\bar{f} \equiv \bar{f}(t,X,\xi)$ denotes the molecular distribution function when written in terms of macroscopic (t,X). The collision operator $I_\xi(\bar{f},\bar{f})$, regarded as a velocity or momentum space operator, is not affected by the change in variables. Equation (27) with $\epsilon = \varepsilon$ simplifies into

$$\frac{\partial \bar{f}}{\partial t} + \xi \cdot \nabla \bar{f} - \epsilon \nabla \cdot \kappa \nabla \bar{f} - \frac{1}{\epsilon} I_\xi(\bar{f},\bar{f}) = 0. \tag{28}$$

This kinetic equation (28) displays some important features that deserve particular attention: for a small local Knudsen number, the collision integral dominates the microscopic spatial diffusion term (which itself becomes negligible). Specifically, for small local Knudsen numbers, this equation is the Boltzmann deterministic equation without a spatial stochastic component [10]. The second important feature is that the spatial diffusion term and the collision integral term vary in opposite ways to each other with regard to changes in the local Knudsen number.

D. Re-interpretation of macroscopic flow properties and the continuum set of equations

The macroscopic flow properties, mass density $\rho(t,X)$, flow velocity $U(t,X)$, and others, are defined in Eqs. (2)–(5), except that now the distribution function is replaced by $\bar{f}(t,X,\xi)$. Multiplying the stochastic kinetic equation (28) by $M, M\xi, M\xi^2/2$ and integrating over velocity space yields the following set of equations:

(1) Mass density,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho U] \underline{- \epsilon \nabla \cdot [\kappa \nabla \rho]} = 0, \tag{29}$$

(2) Momentum,

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot [\rho U U] + \nabla \cdot [p\mathbf{I} + \Pi] \underline{- \epsilon \nabla \cdot [\kappa \nabla (\rho U)]} = 0, \tag{30}$$

(3) Energy,

$$\begin{aligned} &\frac{\partial}{\partial t}\left[\frac{1}{2}\rho U^2 + \rho e_{in}\right] + \nabla \cdot \left[\frac{1}{2}\rho U^2 U + \rho e_{in} U\right] \\ &\quad + \nabla \cdot [(p\mathbf{I} + \Pi) \cdot U] + \nabla \cdot [\mathbf{q}] \\ &\quad \underline{- \epsilon \nabla \cdot \left[\kappa \nabla \left(\frac{1}{2}\rho U^2 + \rho e_{in}\right)\right]} = 0. \end{aligned} \tag{31}$$

Note that this set of equations is the Navier-Stokes-Fourier hydrodynamic model when the local Knudsen number is small, i.e., when $\epsilon \ll 1$. In that hydrodynamic regime, terms related to any volume-mass diffusion vanish. Consequently, we can assert that the set of Eqs. (29)–(31) does not violate the mechanical or thermodynamic consistency existing at the Navier-Stokes-Fourier order. Specifically, with the temporal and spatial scale differences between the micro- and macroscopic clarified in kinetic equation (28), a new entropy

evolution equation results [viz. Eq. (19)]

$$\rho\frac{Ds}{Dt}-\rho\epsilon\kappa c_v\nabla\cdot\left(\frac{\nabla(\rho T)}{\rho T}\right)+\rho\epsilon\kappa(R+c_v)\nabla\cdot\left(\frac{\nabla\rho}{\rho}\right)-\kappa_h\nabla\cdot\left(\frac{\nabla T}{T}\right)$$
$$=\frac{\epsilon\kappa\rho}{T}\nabla U{:}\nabla U-\frac{1}{T}\Pi{:}\nabla U+\frac{\kappa_h+\rho\epsilon\kappa c_v}{T^2}\nabla T\cdot\nabla T+\left\{\frac{2\epsilon\kappa T c_v}{T^2}\nabla\rho\cdot\nabla T-\frac{\epsilon\rho\kappa R}{\rho^2}\nabla\rho\cdot\nabla\rho\right\}. \quad (32)$$

Taking the limit $\epsilon\mapsto 0$, while assuming κ to have a finite value, Eq. (32) yields

$$\rho\frac{Ds}{Dt}-\kappa_h\nabla\cdot\left(\frac{\nabla T}{T}\right)=-\frac{1}{T}\Pi{:}\nabla U+\frac{\kappa_h}{T^2}\nabla T\cdot\nabla T, \quad (33)$$

which is the entropy evolution equation within a conventional Navier-Stokes-Fourier framework without any additional modification. In other words, there is no thermodynamic contradiction. The same observation obtains for angular momentum conservation, when considering Eq. (12) and including the scaling difference.

IV. EXISTENCE OF A CONSISTENT VOLUME-MASS DIFFUSION MODEL AT ORDER $K_{n_{\rm loc}}$

From the previous section, a question that arises is whether it is possible to obtain a hydrodynamic equation that is of first order in $K_{n_{\rm loc}}$ and first order in K_n without violating mechanical properties.

In the original Klimontovich kinetic equation (1), molecular spatial stochasticity has been incorporated exclusively as a spatial diffusion term only. Another way of implementing this physical aspect in the modeling consists of introducing the local volume as an independent microscopic random variable. This rather more complete version of kinetic equation (1) was presented in Ref. [23], and a transport equation was developed for the local volume. The associated set of macroscopic equations, after neglecting nonlinear diffusive fluxes, may be written as follows [24], denoting the material derivative by $D/Dt=\partial/\partial t+U_m\cdot\nabla$:

$$\frac{D\rho}{Dt}=-\rho\nabla\cdot U_m, \quad (34a)$$
$$\rho\frac{DU_m}{Dt}=-\nabla\cdot\mathbf{\Pi}, \quad (34b)$$
$$\rho\frac{D}{Dt}\left[\frac{1}{2}U_m^2+e_{in}\right]=-\nabla\cdot[\mathbf{\Pi}\cdot U_v]-\nabla\cdot\mathbf{J_u}, \quad (34c)$$

closed with

$$\mathbf{\Pi}=p\mathbf{I}+\Pi_{\mathbf{v}},\quad \Pi_{\mathbf{v}}=-2\mu\overline{\overline{\nabla U_v}}^{\circ}, \quad (35a)$$
$$\mathbf{J_u}=-\kappa_h\nabla T, \quad (35b)$$
$$U_v=U_m+\mathbf{J}_v,\quad \mathbf{J}_v=\frac{\kappa_m}{\rho}\nabla\rho, \quad (35c)$$

where

$$\overline{\overline{\nabla U_v}}^{\circ}=\tfrac{1}{2}\left(\nabla U_v+\overline{\nabla U_v}\right)-\tfrac{1}{3}\nabla\cdot U_v\mathbf{I}. \quad (36)$$

A single bar over the velocity gradient here denotes the transpose operator, and $\mathbf{I}$ is the second order identity tensor. In the above set of equations, the volume-mass diffusive flux is $\mathbf{J}_v$ in Eq. (35c). It appears primarily through the expression of the shear stress, Eq. (35a), and is associated with another form of velocity U_v termed the volume velocity [23]. Velocity U_m, used in the material derivative, is the traditional mass current velocity, giving the mass flux and satisfying the continuity equation (34a). The additional transport coefficient κ_m is the volume-mass diffusivity coefficient.

Taking the cross product of Eq. (34b) with hydrodynamic position vector X,

$$X\wedge\rho\frac{DU_m}{Dt}=-X\wedge\nabla\cdot[p\mathbf{I}+\mathbf{\Pi}_v], \quad (37)$$

which is equivalent to

$$\rho\frac{D}{Dt}[X\wedge U_m]=-X\wedge\nabla\cdot[p\mathbf{I}+\mathbf{\Pi}_v]. \quad (38)$$

For any symmetrical second order tensor $\bar{\bar{\mathrm{T}}}$, the following property holds:

$$X\wedge[\nabla\cdot\bar{\bar{\mathrm{T}}}]=\nabla\cdot[X\wedge\bar{\bar{\mathrm{T}}}], \quad (39)$$

and the pressure tensor $\mathbf{\Pi}_v$ given in Eq. (35a) is symmetrical. So, Eq. (38) has the following final form:

$$\rho\frac{D}{Dt}[X\wedge U_m]=-\nabla\cdot[X\wedge[p\mathbf{I}+\Pi_{\mathbf{v}}]]. \quad (40)$$

Therefore, conservation of angular momentum is satisfied. More generally, it is also straightforward to verify that the hydrodynamic set of Eqs. (34a)–(35c) satisfies mechanical properties, such as Galilean invariance, integrability, angular momentum conservation, and center-of-mass position (see Ref. [24]). The principal reason for this is that the mass flux velocity vector U_m in Eq. (34a) is the same as that in the momentum density on the left-hand side of Eq. (34b). In contrast, note that velocity vector U, within the set of Eqs. (6)–(8), is comparable with U_v in Eq. (35c) and not the mass current velocity U_m. This distinction is crucial to interpret angular momentum conservation and other mechanical properties appropriately. In Ref. [24], the second law of thermodynamics is also shown through an extended thermodynamics approach (however, see also Refs. [25–27]). The momentum equation (34b), closed with Eq. (35a), is the same as that derived by Koide and Kodama using an explicit stochastic approach [28]. In the Appendix, we give another example showing the important role played by the spatial scaling.

V. DISCUSSION

The distinction we have made between $K_{n_{\rm loc}}$ and K_n separates local relaxation processes not related to momentum

diffusion from relaxation processes related to momentum diffusion. Momentum diffusion and heat diffusion are both associated with collisions: the shear stress and heat flux of the Navier-Stokes-Fourier model are first order in the traditional Knudsen number K_n. In our case, volume-mass diffusion appears as another form of transport process driven by spatial stochastic behaviors rather than intermolecular collisions, and so is a nonequilibrium effect we quantify using $K_{n_{\text{loc}}}$ at a fixed K_n.

The slip and transition flow regimes correspond primarily to relatively large mean-free-path regimes where the flow is still under the classical assumption of $l_{\text{loc}} \ll L$. Diffusive volume-mass models are reported as producing better agreement with experiments for these types of flow problems [6–9,18]. Our description and the new classification in Sec. III appear to shed some light on this issue. Volume-mass diffusion appears simply as a component of the flow physics, originating from a different order of the microstructure behavior. It appears in addition to and alongside traditional heat and momentum diffusion processes.

Equation (28) has a strong similarity not only in its form, but also in its derivation to the (extended) Boltzmann kinetic equation that leads to the "ghost effect" (i.e., where high Knudsen number terms are found to influence flows in the hydrodynamic or pure continuum regime [20]). The (apparent) inconsistency observed when using hydrodynamic models associated with the Klimontovich kinetic equation (1) may be understood because that description did not identify the distinction between the "mass velocity" and the "volume or diffusion velocity," which are related, respectively, to "mass averaging" and "volume averaging" [29].

It is widely known that, when conducting a Chapman-Enskog type of expansion in K_n on the Boltzmann kinetic equation without any spatial diffusion modification, the second order hydrodynamic model beyond that of Navier-Stokes-Fourier, namely, the Burnett equations, violates many conventional mechanical and thermodynamical properties [14–17]. We note that the volume-mass diffusion contributions in our hydrodynamic set of equations [for example, in the momentum equation (34b)] are also of Burnett order. These contributions are identical to corrective terms to the Navier-Stokes equations that produce the "ghost effect" [30]. A hydrodynamic set of equations [such as the set (34a)–(35c)], which maintains mechanical and thermodynamic consistencies while containing Burnett order terms, is a significant result from the kinetic theory point of view.

VI. CONCLUSION

We have shown that diffusive volume (or mass), as a component of models for non-continuum flows, does not conflict thermodynamically or mechanically with the Navier-Stokes-Fourier model, provided micro- and macroscopic time and space scales are distinguished in the governing equations. There appears to be a subdomain in the continuum range for which the conventional Knudsen number classification does not properly account for. Classical diffusive transports, i.e., shear stress and heat flux, are vanishing local Knudsen number effects, whereas, volume or mass diffusion appears at different but parallel orders. Volume-mass diffusion is simply another level of microstructure contributions beyond that of the Navier-Stokes-Fourier diffusion processes. Its emergence at a finite Knudsen number at least partly explains the perplexingly good agreement of these new models with the experiments on noncontinuum flows.

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APPENDIX: THE SPATIAL SCALING PROBLEM FROM THE VIEWPOINT OF A KINETIC MODEL INCORPORATING STOCHASTIC MOLECULAR MOTION

In Refs. [31,32], a kinetic equation is proposed that consists of replacing the Boltzmann collision integral with a velocity space stochastic operator. The proposed kinetic equation is written

$$\frac{\partial \mathfrak{f}}{\partial t} + V_i \frac{\partial \mathfrak{f}}{\partial x_i} = \mathfrak{S}(\mathfrak{f}), \tag{A1}$$

where $\mathfrak{S}(\mathfrak{f})$, the proposed velocity space stochastic operator, reads

$$\mathfrak{S}(\mathfrak{f}) = -\frac{\partial A_i \mathfrak{f}}{\partial V_i} + \frac{D^2}{2} \frac{\partial^2 \mathfrak{f}}{\partial V_j \partial V_j}, \tag{A2}$$

with $\mathfrak{f} \equiv \mathfrak{f}(t,x,V)$ as the molecular distribution probability density function. Coefficient D and vector A are given the expressions [32],

$$A_i = -\frac{1}{\tau}(V_i - U_i) \quad \text{and} \quad \frac{D^2}{2} = \frac{2e_{in}}{3\tau}, \tag{A3}$$

with U as a gas macroscopic velocity, τ as a relaxation time, and V is the molecular velocity. The distribution function $\mathfrak{f}$ in Eq. (A1) is primarily a function of the macroscopic time and spatial position variables, denoted t and x, respectively (see p. 4 of Ref. [32]).

The authors then assumed that kinetic model (A1) is equivalent to the following coupled stochastic molecular motion equations:

$$\begin{aligned} \frac{\delta X_i}{\delta t} &= M_i, \\ \frac{\delta M_i}{\delta t} &= -\frac{1}{\tau}(M_i - U_i) + \left(\frac{4e_{in}}{3\tau}\right)^{1/2} \frac{\delta\, \mathrm{Wi}(t)}{\delta t}, \end{aligned} \tag{A4}$$

where X_i refers to molecule positions, M_i refers to molecule velocities, and $\mathrm{Wi}(t)$ is a Wiener process representing the stochastic force component.

In the coupled equations (A4), we first note that the position variable X_i and velocity variable M_i are no longer independent but rather are coupled. Second, the position variable (and the time variable) in Eq. (A4) is not the same as the position (or time) variable in Eq. (A1). This crucial point was recognized by the authors as they denoted one of these variables x and the other X (see p. 8 of Ref. [32]). Finally, in stochastic

equations, such as Eq. (A4), derivative operators are no longer ordinary derivatives but should be treated in the Ito sense. That is to say, we need a definition of a measure and the use of the Ito integration formula. This explicit integration has been performed by Bogomolov and Dorodnitsyn [10], who derived the macroscopic set of equations from Eq. (A4). Taking into account the fact that position is given by the time integral of the velocity and the Ito transformation, they gave for the macroscopic fluid density the following equation [10]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left[\rho U - \frac{1}{2} K_{n_{\mathrm{loc}}} \frac{D^2}{A^2} \nabla \rho \right] = 0, \tag{A5}$$

which is a dissipative volume-mass type of equation for the density. Note that the diffusive term in Eq. (6) is derived directly from the second term in the Ito formula. Physically, it is just the translation of the stochasticity implemented on the velocity in Eq. (A4) onto particle positions. Parameter $K_{n_{\mathrm{loc}}}$ is the signature of the transition from variable X to variable x: it is a local Knudsen number in the same way as in our Eq. (23). Associating a transition measure between variables x and X was the same source that led previously to the Klimontovich kinetic equation.

Gorji *et al.* [32] reported very good agreement of their stochastic kinetic equation (A4) with experiments for a slip or transition regime flow as did Bogomolov and Dorodnitsyn [10].

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